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December 2, 2005

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Commissioner for Patents  
PO Box 1450  
Alexandria, VA 22313-1450

*Art Unit 2857*

*Attn: Mail Stop Amendment*

Re: U.S. Utility Patent Application  
Application No.: 10/791,681; Filed: March 3, 2004  
For: **Methods and Systems for Preparing Virtual Representations of Molecules**

Inventor: Frank P. HOLLINGER, Ph.D.  
Our Ref: 1866.0220001/PEG/CMB

Sir:

Transmitted herewith for appropriate action are the following documents:

1. Information Disclosure Statement Filing Under 37 C.F.R. § 1.97(b);
2. Form PTO/SB/08A listing twenty-one (21) cited references (1 page);
3. Copies of five (5) of the twenty-one (21) cited references;
4. Form PTO/SB08B listing sixty-nine (69) cited references (7 pages);
5. Copies of sixty-six (66) of the sixty-nine (69) cited references; and
6. One (1) return postcard.

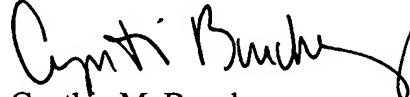
It is respectfully requested that the attached postcard be stamped with the date of filing of these documents, and that it be returned to our courier. In the event that extensions of time are necessary to prevent abandonment of this patent application, then such extensions of time are hereby petitioned.

Commissioner for Patents  
December 2, 2005  
Page 2

The U.S. Patent and Trademark Office is hereby authorized to charge any fee deficiency, or credit any overpayment, to our Deposit Account No. 19-0036.

Respectfully submitted,

STERNE, KESSLER, GOLDSTEIN & FOX P.L.L.C.



Cynthia M. Bouchez  
Attorney for Applicant  
Registration No. 47,438

PEG/CMB:krh  
Enclosures

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IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

In re application of:

Frank P. Hollinger

Appl. No.: 10/791,681

Filed: March 3, 2004

For: **Methods and Systems for  
Preparing Virtual Representations  
of Molecules**

Confirmation No.: 2609

Art Unit: 2857

Examiner: Zeman, Mary K.

Atty. Docket: 1866.0220001/PEG/CMB

**Information Disclosure Statement  
Filing Under 37 C.F.R. § 1.97(b)**

*Mail Stop Amendment*

Commissioner for Patents  
PO Box 1450  
Alexandria, VA 22313-1450

Sir:

Listed on accompanying Form PTO/SB/08A and Form PTO/SB/08B are documents that may be considered material to the examination of this application, in compliance with the duty of disclosure requirements of 37 C.F.R. §§ 1.56, 1.97 and 1.98. Copies of documents **FP1-FP5** and **NPL1-NPL66** are submitted herewith. However, in accordance with 37 C.F.R. § 1.98(a)(2), copies of U.S. patents and patent application publications, documents **US1-US16**, cited on the attached Form PTO/SB/08A are not submitted.

In addition, copies of documents **NPL67-NPL69** are not provided in accordance with the U.S. Patent and Trademark Office OG notice of October 19, 2004, which states: "the requirement in 37 C.F.R. § 1.98(a)(2)(iii) for a legible copy of the specification, including the claims, and drawings of each cited pending U.S. patent application (or

portion of the application which caused it to be listed) is sua sponte waived where the cited pending application is stored in the USPTO's IFW system."

The Examiner's attention is directed to the following U.S. Patent Applications, which are directed to related technical subject matter:

Co-pending U.S. Patent Application No. 11/146,417, inventors Guarnieri, F., *et al.*, filed June 7, 2005, cited herein as document **NPL67**;

Co-pending U.S. Patent Application No. 09/722,731, inventor Guarnieri, F., filed November 28, 2000 not yet published, cited herein as document **NPL68**;

Co-pending U.S. Patent Application No. 10/813,553, inventors Ludington, J., *et al.*, filed March 31, 2004, not yet published, cited herein as document **NPL69**;

Co-pending U.S. Patent Application No. 10/794,181, inventors Brunner, S., *et al.*, filed March 8, 2004, now published as 2004/0267456 A1, cited herein as document **US15**; and

Co-pending U.S. Patent Application No. 10/920,234, inventors Brunner, S., *et al.*, filed August 18, 2004, now published as 2005/0123995 A1, cited herein as document **US16**.

In accordance with the recent Federal Circuit decision in *Dayco Prods., Inc. v. Total Containment, Inc.* 329 F.3d 1358 (Fed. Cir. 2003), Applicants submit herewith Office Actions, which are also directed to related technical subject matter:

Office Action for related U.S. Patent Application No. 09/183,267, inventor Guarnieri, F., filed October 30, 1998, mailed June 30, 2000, cited herein as document **NPL59**;

Office Action for related U.S. Patent Application No. 09/183,267, inventor Guarnieri, F., filed October 30, 1998, mailed March 5, 2001, cited herein as document **NPL60**;

Office Action for related U.S. Patent Application No. 09/183,267, inventor Guarnieri, F., filed October 30, 1998, mailed March 12, 2003, cited herein as document **NPL61**;

Office Action for related U.S. Patent Application No. 09/722,731, inventor Guarnieri, F., filed November 28, 2000, mailed September 26, 2002, cited herein as document **NPL62**; and

Office Action for related U.S. Patent Application No. 09/722,731, inventor Guarnieri, F., filed November 28, 2000, mailed August 30, 2005, cited herein as document **NPL63**.

The identification of these U.S. Patent Applications and Office Actions is not to be construed as a waiver of secrecy as to those applications now or upon issuance of the present application as a patent. The Examiner is respectfully requested to consider the cited applications and the art cited therein during examination.

Where the publication date of a listed document does not provide a month of publication, the year of publication of the listed document is sufficiently earlier than the effective U.S. filing date and any foreign priority date so that the month of publication is not in issue. Applicants have listed publication dates on the attached Form PTO/SB/08A and Form PTO/SB/08B based on information presently available to the undersigned. However, the listed publication dates should not be construed as an admission that the information was actually published on the date indicated.

Applicants reserve the right to establish the patentability of the claimed invention over any of the information provided herewith, and/or to prove that this information may not be prior art, and/or to prove that this information may not be enabling for the teachings purportedly offered.

This statement should not be construed as a representation that a search has been made, or that information more material to the examination of the present patent application does not exist. The Examiner is specifically requested not to rely solely on the material submitted herewith.

This Information Disclosure Statement is being filed before the mailing date of a first Office Action on the merits. No statement or fee is required.

It is respectfully requested that the Examiner initial and return copies of the enclosed Form PTO/SB/08A and Form PTO/SB/08B, and indicate in the official file wrapper of this patent application that the documents have been considered.

The U.S. Patent and Trademark Office is hereby authorized to charge any fee deficiency, or credit any overpayment, to our Deposit Account No. 19-0036.

Respectfully submitted,

STERNE, KESSLER, GOLDSTEIN & FOX P.L.L.C.



Cynthia M. Bouchez  
Attorney for Applicants  
Registration No. 47,438

Date: Dec. 2, 2005

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**INFORMATION DISCLOSURE  
STATEMENT BY APPLICANT**

*(Use as many sheets as necessary)*

*(Use as many sheets as necessary)*

Sheet

1 of 1

*Complete if Known*

Application Number	10/791,681
Filing Date	March 3, 2004
First Named Inventor	Hollinger, Frank
Art Unit	2857
Examiner Name	Zeman, Mary K.
Attorney Docket Number	1866.0220001/PEG/CMB

U.S. PATENT DOCUMENTS

U.S. PATENT DOCUMENTS				
Examiner Initials*	Cite No. <sup>1</sup>	Document Number	Publication Date	Name of Patentee or Applicant of Cited Document
		Number-Kind Code <sup>2</sup> (If Known)	MM-DD-YYYY	
	US1	5,557,535	09/17/1996	Srinivasan et al.
	US2	5,600,571	02/04/1997	Friesner et al.
	US3	5,854,992	12/29/1998	Shakhnovich et al.
	US4	5,884,230	03/16/1999	Srinivasan et al.
	US5	6,029,114	02/22/2000	Shamovsky et al.
	US6	6,178,384 B1	01/23/2001	Kolossvåry
	US7	6,251,620 B1	06/26/2001	Hatada et al.
	US8	6,341,256 B1	01/22/2002	Deem et al.
	US9	6,426,205 B1	07/30/2002	Tyers and Willems
	US10	6,489,608 B1	12/03/2002	Silling
	US11	6,640,191 B1	10/28/2003	Deem et al.
	US12	6,716,614 B1	04/06/2004	Donoho et al.
	US13	6,735,530 B1	05/11/2004	Guarnieri
	US14	2003/0055574 A1	03/20/2003	Still et al.
	US15	2004/0267456 A1	12/30/2004	Brunner et al.
	US16	2005/0123995 A1	06/09/2005	Brunner et al.

## **FOREIGN PATENT DOCUMENTS**

CITED PATENT DOCUMENTS				
Examiner Initials*	Cite No. <sup>1</sup>	Foreign Patent Document	Publication Date MM-DD-YYYY	Name of Patentee or Applicant of Cited Document
		Country Code <sup>3</sup> Number <sup>4</sup> Kind Code <sup>5</sup> (if known)		
	FP1	WO 96/34347 A1	10/31/1996	Mount Sinai School of Medicine of the City University of New York and Guarnieri
	FP2	WO 97/16177 A1	05/09/1997	SmithKline Beecham Corporation and Abdel-Meguid <i>et al.</i>
	FP3	EP 0 807 687 A2	11/19/1997	SmithKline Beecham Corporation and Abdel-Meguid <i>et al.</i>
	FP4	WO 04/081841 A1	09/23/2004	Sarnoff Corporation and Guanieri
	FP5	WO 04/078932 A2	09/16/2004	Locus Pharmaceuticals, Inc. and Hollinger

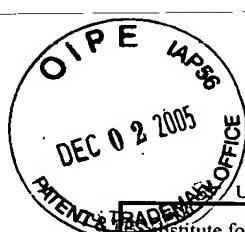
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## INFORMATION DISCLOSURE STATEMENT BY APPLICANT

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Sheet 1 of 7

**Complete if Known**

Application Number	10/791,681
Filing Date	March 3, 2004
First Named Inventor	Hollinger, Frank
Art Unit	2857
Examiner Name	Zeman, Mary K

Attorney Docket Number 1866.0220001/PEG/CMB

**NON PATENT LITERATURE DOCUMENTS**

Examiner Initials*	Cite No. <sup>1</sup>	Include name of the author (in CAPITAL LETTERS), title of the article (when appropriate), title of the item (book, magazine, journal, serial, symposium, catalog, etc.), date, page(s), volume number, publisher, city and/or country where published	T <sup>2</sup>
	NPL1	Adachi, M., et al., "A novel methodology for assisting in the discovery of new chromogens: theoretical calculations with high throughput screening," <i>Advances in Colour Science and Technology</i> 4:124-129, University of Leeds (2001)	
	NPL2	Adams, D.J., "Grand canonical ensemble Monte Carlo for a Lennard-Jones fluid," <i>Mol. Phys.</i> 29:307-311, Taylor & Francis Ltd. (1975)	
	NPL3	Apostolakis, J., et al., "Computational Ligand Design," <i>Combinatorial Chemistry and High Throughput Screening</i> 2:91-104, Bentham Science Publishers B.V. (1999)	
	NPL4	Basson, I. and Reynhardt, E.C., "NMR of montan wax," <i>J. Phys. D: Appl. Phys.</i> 21:1434-1437, IOP Publishing Ltd. (1998)	
	NPL5	Basson, I. and Reynhardt, E.C., "An investigation of the structures and molecular dynamics of natural waxes: III. Montan wax," <i>J. Phys. D: Appl. Phys.</i> 21:1434-1437, IOP Publishing Ltd. (1988)	
	NPL6	Blaskó, A., et al., "Pendant-Capped Porphyrins.2. Structural Analysis and Dynamics of the Biphenyl Pendant-Capped Porphyrin Model of Catalase and Its Fe (III) Complex by One- and Two-Dimensional 1H NMR Spectroscopy and Distance Geometry/Molecular Modeling Refinement," <i>J. Am. Chem.</i> 58:5738-5747, American Chemical Society (1993)	
	NPL7	Brandmeier, V., et al., "8. Antiparallel $\beta$ -Sheet Conformation in Cyclopeptides Containing a Pseudo-amino Acid with Biphenyl Moiety," <i>Helv. Chim. Acta</i> 77:70-85, Neu Schweizerische Chemische Gesellschaft (1994)	
	NPL8	Bredikhin, A., et al., "Molecular and Crystalline Structure of Dimethyl 4,6-Dimethyl-2-(2-nitrophenyl)-1,2-dihydropyridine-3,5-dicarboxylate, By-product in the Synthesis of Nifedipine," <i>Russian Journal of Organic Chemistry</i> 35:1372-1376, Minsk "Hayka/Interperiodica" (1999)	
	NPL9	Cafisch, A., et al., "Multiple Copy Simultaneous Search and Construction of Ligands in Binding Sites: Application to Inhibitors of HIV-1 Aspartic Proteinase," <i>J. Med. Chem.</i> 36:2142-2167, American Chemical Society (1993)	
	NPL10	Calafat, A.M., et al., "A New Arrangement for the Anticancer Antibiotics Tallysomycin and Bleomycin When Bound to Zinc: An Assessment of Metal and Ligand Chirality by NMR and Molecular Dynamics," <i>J. Am. Chem. Soc.</i> 119:3656-3664, American Chemical Society (1997)	

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				Application Number	10/791,681
				Filing Date	March 3, 2004
				First Named Inventor	Hollinger, Frank
				Art Unit	2857
				Examiner Name	Zeman, Mary K
Sheet	2	of	7	Attorney Docket Number	1866.0220001/PEG/CMB

<b>NON PATENT LITERATURE DOCUMENTS</b>					
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	NPL11	Catlow, C., et al., "Computer Modeling of Nucleation, Growth, and Templating in Hydrothermal Synthesis," <i>Chem. Mater.</i> 10:3249-3265, American Chemical Society (1998)			
	NPL12	Clough, S.B., et al., "Molecular Dynamics Simulation of Substituted Conjugated Ionic Polyacetylenes," <i>Macromolecules</i> 26:597-600, American Chemical Society (1993)			
	NPL13	Chan, D.C., et al., "Core Structure of gp41 from the HIV Envelope Glycoprotein," <i>Cell</i> 89:263-273, Cell Press (1997)			
	NPL14	Chen, B., et al., "Synthesis of Specifically Deuterated Nucleotides and Their Application in Mechanistic Elucidation of DNA and RNA Cleavage by the Hydroxyl Radical," Abstract No. 116, Book of Abstracts, American Chemical Society, 224th ACS National Meeting, Boston, MA (August 18-22, 2002)			
	NPL15	Dennis, S., et al., "Computational mapping identifies the binding sites of organic solvents on proteins," <i>Proc. Natl. Acad. Sci. USA</i> 99:4290-4295, National Academy of Sciences (April 2002)			
	NPL16	Ding, X., et al., "Nature of the Inactivation of Elastase by N-Peptidyl O aryl hydroxylamine as a Function of pH," <i>Biochem.</i> 34:7749-7756, American Chemical Society (1995)			
	NPL17	Duggan, H. and Craik, D.J., " <sup>1</sup> H and <sup>13</sup> C NMR Relaxation Studies of Molecular Dynamics of the Thyroid Hormones Thyroxine, 3, 5, 3'-Triiodothyronine, and 3,5,-Diiodothyronine," <i>J. Med. Chem.</i> 39:4007-4016, American Chemical Society (1996)			
	NPL18	Edwards and Burnstein, "Synthetic Inhibitors of Elastase," <i>Med. Res. Rev.</i> 14:127-194, John Wiley & Sons, Inc. (1994)			
	NPL19	Gibson, K.D. and Scheraga, H.A., "Crystal Packing without Symmetry Constraints.2. Possible Crystal Packings of Benzene Obtained by Energy Minimization from Multiple Starts," <i>J. Phys. Chem.</i> 99:3765-3773, American Chemical Society (1995)			
	NPL20	Guarnieri, F., and Mezei, M., "Simulated Annealing of Chemical Potential: A General Procedure for Locating Bound Waters. Application to the Study of the Differential Hydration Propensities of the Major and Minor Grooves of DNA," <i>J. Am. Chem. Soc.</i> 118:8493-8494, American Chemical Society (1996)			

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	NPL21	Henson, N., et al., "Computational Studies of Cobalt-Substituted Aluminophosphates," <i>J. Phys. Chem. A</i> 104:2423-2431, American Chemical Society (2000)			
	NPL22	Honma, T., "Recent Advances in De Novo Design Strategy for Practical Lead Identification," <i>Med. Res. Rev.</i> 23:606-632, Wiley Periodicals, Inc. (September 2003)			
	NPL23	Huang, C.C., et al., "Integrated Tools for Structural and Sequence Alignment and Analysis," <i>Pacific Symposium on Biocomputing</i> , presented at the <i>Pacific Symposium on Biocomputing</i> , Oahu, Hawaii, pp.230-241 (2000)			
	NPL24	Johnson, P.M., "Resonance ionization spectra as a reflection of excited state dynamics," <i>Inst. Phys. Conf. Ser. No 114: Section 4:145-150</i> , presented at the <i>Proceedings of the Fifth International Symposium on Resonance Ionization Spectroscopy and its Applications</i> , Congress Centre Villa Ponti, Varese, Italy (1990)			
	NPL25	Joseph-McCarthy, D., et al., "Use of MCSS to Design Small Targeted Libraries: Application to Picornavirus Ligands," <i>J. Am. Chem. Soc.</i> 123:12758-12769, American Chemical Society (2001)			
	NPL26	Koone, N., et al., "Diffusion of Simple Liquids in Porous Sol-Gel Glass," <i>J. Phys. Chem.</i> 99:16976-16981, American Chemical Society (1995)			
	NPL27	Kortemme, T., and Baker, D., "A simple physical model for binding energy hot spots in protein-protein complexes," <i>Proc. Natl. Acad. Sci. USA</i> 99:14116-14121, National Academy of Sciences (October 2002)			
	NPL28	Lee, T. and Jones, J.B., "Probing the Abilities of Synthetically Useful Serine Proteases to Discriminate between the Configurations of Remote Stereocenters Using Chiral Aldehyde Inhibitors," <i>J. Am. Chem. Soc.</i> 118:502-508, American Chemical Society (1996)			
	NPL29	Lee, Y.-C., et al., "Computational Studies of the Silicon Substitution Effects in Polyelectrolytes Containing Zeolitic Fragments," <i>Polymeric Materials Science and Engineering</i> 80:620-621, American Chemical Society (1999)			
	NPL30	Lee, Y.-C., et al., "Computational Studies of Polyelectrolytes Containing Zeolitic Fragments," <i>J. Phys. Chem. B</i> 103:6445-6449, American Chemical Society (1999)			

Examiner Signature		Date Considered	
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Substitute for form 1449/PTO				<b>Complete if Known</b>	
<b>INFORMATION DISCLOSURE STATEMENT BY APPLICANT</b> <i>(Use as many sheets as necessary)</i>				Application Number	10/791,681
				Filing Date	March 3, 2004
				First Named Inventor	Hollinger, Frank
				Art Unit	2857
				Examiner Name	Zeman, Mary K
Sheet	4	of	7	Attorney Docket Number	1866.0220001/PEG/CMB

<b>NON PATENT LITERATURE DOCUMENTS</b>				
Examiner Initials*	Cite No. <sup>1</sup>	Include name of the author (in CAPITAL LETTERS), title of the article (when appropriate), title of the item (book, magazine, journal, serial, symposium, catalog, etc.), date, page(s), volume number, publisher, city and/or country where published		T <sup>2</sup>
	NPL31	Lynch and Pettit, "Grand canonical ensemble molecular dynamics simulations: Reformulation of extended system dynamics approaches," <i>J. Chem. Phys.</i> 107:8594-8610, American Chemical Society (1997)		
	NPL32	Lunazzi, L., et al., "Conformational Studies by Dynamic NMR, 58. <sup>1</sup> Steeodynamics of C-C and C-N Rotation in Furan and Thiophene o-Amino Thioaldehydes and Aldehydes," <i>J. Org. Chem.</i> 62:2263-2266, American Chemical Society (1997)		
	NPL33	Massova, I., and Kollman, P.A., "Computational Alanine Scanning to Probe Protein Protein Interactions: A Novel Approach To Evaluate Binding Free Energies," <i>J. Am. Chem. Soc.</i> 121:8133-8143, American Chemical Society (1999)		
	NPL34	Mattos, C., et al., "Analogous inhibitors of elastase do not always bind analogously," <i>Struct. Biol.</i> 1:55-58, Nature Publishing Company (1994)		
	NPL35	Mattos, C., et al., "Structural Analysis of the Active Site of Porcine Pancreatic Elastase Based on the X-ray Crystal Structures of Complexes with Trifluoroacetyl- Dipeptide-Anilide Inhibitors," <i>Biochemistry</i> 34:3193-3203, American Chemical Society (1995)		
	NPL36	Mehler, E.L. and Guarnieri, F., "A Self-Consistent, Microenvironment Modulated Screened Coulomb Potential Approximation to Calculate pH-Dependent Electrostatic Effects in Proteins," <i>Biophys. J.</i> 75:3-22, Biophysical Society (1999)		
	NPL37	Mehrotra, P.K. and Beveridge, D.L., "Structural Analysis of Molecular Solutions Based on Quasi-Component Distribution Functions. Application to [H <sub>2</sub> O] <sub>aq</sub> at 25°C," <i>J. Am. Chem. Soc.</i> 102:4287-4294, American Chemical Society (1980)		
	NPL38	Metropolis, N., et al., "Equation of State Calculations by Fast Computing Machines," <i>J. Chem. Phys.</i> 21:1087-1092, American Institute of Physics (1953)		
	NPL39	Mezei, M., "Grand-canonical ensemble Monte Carlo study of dense liquid Lennard-Jones, soft spheres and water," <i>Mol. Phys.</i> 61:565-582, Taylor & Francis Ltd. (1987)		
	NPL40	Mezei, M. and Beveridge, D.L., "Structural Chemistry of Bimolecular Hydration via Computer Simulation: The Proximity Criterion," in <i>Methods in Enzymology</i> , Packer, ed., Academic Press, NY, pp. 21-47, (1986)		

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				Examiner Name	Zeman, Mary K
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	NPL41	Mezei, M., "Modified Proximity Criteria for the Analysis of the Solvation of a Polyfunctional Solute," <i>Mol. Simul.</i> 1:327-332, Gordon and Breach Science Publishers S.A. (1988)			
	NPL42	Mezey, P., "Relations between Computational and Experimental Engineering Approaches to Molecules from Molecular Fragments," <i>Molecular Engineering</i> 8:235-250, Kluwer Academic Publishers (1999)			
	NPL43	Miranker, A., and Karplus, M., "Functionality Maps of Binding Sites: A Multiple Copy Simultaneous Search Method," <i>Proteins</i> 11:29-34, Wiley-Liss, Inc. (1991)			
	NPL44	Mokrosz, J.L., et al., "Conformational Analysis of 4-(2'-Furyl)-2-(methylamino) pyrimidine," <i>J. Heterocyclic Chem.</i> 33:1207-1210, HeteroCorporation (1996)			
	NPL45	Morgantini, P.-Y. and Kollman, P.A., "Solvation Free Energies of Amides and Amines: Disagreement between Free Energy Calculations and Experiment," <i>J. Am. Chem. Soc.</i> 117:6057-6063, American Chemical Society (1995)			
	NPL46	Ondrechen, M.J., et al., "THEMATICS: A simple computational predictor of enzyme function from structure," <i>Proc. Natl. Acad. Sci. USA</i> 98:12473-12478, The National Academy of Sciences (2001)			
	NPL47	Petoukhov et al., "Addition of Missing Loops and Domains to Protein Models by X-Ray-Solution Scattering," <i>Biophys. J.</i> 83:3113-3125, Biophysical Society (December 2002)			
	NPL48	Raineri, F.O., et al., "Surrogate Hamiltonian description of solvation dynamics. Resolution of global responses into spatial profiles," <i>Chem. Phys.</i> 183:187-205, Elsevier Science B.V. (1994)			
	NPL49	Resat, H. and Mezei, M., "Grand Canonical Ensemble Monte Carlo Simulation of the dCpG/Proflavine Crystal Hydrate," <i>Biophys. J.</i> 71:1179-1190, Biophysical Society (1996)			
	NPL50	Resat, H. and Mezei, M., "Grand canonical Monte Carlo Simulation of Water Positions in Crystal Hydrates," <i>J. Am. Chem. Soc.</i> 116:7451-7452, American chemical Society (1994)			

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	NPL51	Resat, H., et al., "Use of the Grand Canonical Ensemble in Potential of Mean Force Calculations," <i>J. Phys. Chem.</i> 100:1426-1433, American Chemical Society (1996)		
	NPL52	Siepmann, J.I. and McDonald, I.R., "Monte Carlo study of the properties of self-assembled monolayers formed by adsorption of CH <sub>3</sub> (CH <sub>2</sub> ) <sub>15</sub> SH on the (111) surface of gold," <i>Mol. Phys.</i> 79:457-473, Taylor and Francis Ltd. (1993)		
	NPL53	Vaidehi, N., et al., "Prediction of structure and function of G protein-coupled receptors," <i>Proc. Natl. Acad. Sci.</i> 99:12622-12627, National Academy of Sciences (October 2002)		
	NPL54	Verkhivker, G.M., et al., "Monte Carlo Simulations of the Recognition at the Consensus Binding Site of the Constant Fragment of Human Immunoglobulin G: the Energy Landscape Analysis of a Hot Spot at the Intermolecular Interface," <i>Proteins: Structure, Function, and Genetics</i> 48:539-557, Wiley-Liss, Inc. (August 2002)		
	NPL55	International Search Report for International Application No. PCT/US2003/07366, IPEA, Alexandria, VA, mailed on May 25, 2005		
	NPL56	International Search Report for International Application No. PCT/US2003/07366, International Search Authority, Alexandria, VA, mailed on October 30, 2003		
	NPL57	International Search Report for International Application No. PCT/US2004/06347, International Search Authority, Alexandria, VA, mailed on April 12, 2005		
	NPL58	International Search Report for International Application No. PCT/US2004/14069, International Search Authority, Alexandria, VA, mailed on October 8, 2004		
	NPL59	Copy of Office Action for U.S. Patent Application No. 09/183,267, inventor Guarnieri, F., filed October 30, 1998, mailed on June 30, 2000		
	NPL60	Copy of Office Action for U.S. Patent Application No. 09/183,267, inventor Guarnieri, F., filed October 30, 1998, mailed on March 5, 2001		

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	NPL61	Copy of Office Action for U.S. Patent Application No. 09/183,267, inventor Guarnieri, F., filed October 30, 1998, mailed on March 12, 2003		
	NPL62	Copy of Office Action for U.S. Patent Application No. 09/722,731, inventor Guarnieri, F., filed November 28, 2000, mailed on September 26, 2002		
	NPL63	Copy of Office Action for U.S. Patent Application No. 09/722,731, inventor Guarnieri, F., filed November 28, 2000, mailed on August 30, 2005		
	NPL64	Goodsell, D.S. and Olson, A.J., "Automated Docking of Substrates to Proteins by Simulated Annealing," <i>Proteins: Structure, Function, and Genetics</i> 8:195-202, Wiley-Liss, Inc. (1990)		
	NPL65	Meng, E.C., et al., "Automated Docking with Grid-Based Energy Evaluation," <i>J. Comp. Chem.</i> 13:505-524, John Wiley & Sons, Inc. (1992)		
	NPL66	Nilges, M., et al., "Determination of three-dimensional structures of proteins from interproton distance data by dynamical simulated annealing from a random array of atoms," <i>FEBS Lett.</i> 239:129-136, Elsevier Science Publishers B.V. (1988)		
	NPL67	Co-pending U.S. Provisional Application No. 11/146,417, inventors Guarnieri, F., et al., filed June 7, 2005 (NOT PUBLISHED)		
	NPL68	Co-pending U.S. Application No. 09/722,731, inventor Guarnieri, F., filed November 28, 2000 (NOT PUBLISHED)		
	NPL69	Co-pending U.S. Application No. 10/813,553, inventors Ludington, J., et al., filed March 31, 2004 (NOT PUBLISHED)		

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